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Sputtering by a sum of impulses: The effect of finite track width

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A continuum mechanical model of the effect of the pressure pulse produced by a sudden deposition of energy inside a cylindrical track in a solid (e.g., by an energetic ion) is extended to cases with finite track width.

Heavy energetic ions penetrating solids deposit their energy in a roughly cylindrical track. Due to the large energy gradients around the track, material can be ejected from the solid. A continuum mechanical approach has been described[1] and has been used to calculate the ejection yield as a function of the deposited energy for comparison with molecular-dynamics simulations[2,3] and experiments.[4] These calculations were all done under the assumption that the energy is deposited in a track with a radial extension much smaller than the ejected volume. Because of the usefulness of the continuum mechanical model which has earlier been demonstrated by comparison with molecular-dynamics simulations,[2,3] the model is extended to cases with finite track width in this Brief Report.

The energy deposited in the solid by the incoming ion is assumed to spread according to

$$\frac{d\varepsilon(\mathbf{r},t)}{dt}=\nabla\cdot[\kappa\nabla\varepsilon(\mathbf{r},t)]\ , \tag{1}$$

where ε is the energy density, r is the position in the solid, t is the time, and κ is the diffusivity. The solution for constant κ and a line of point sources of energy, i.e., zero track width, extending from the surface a distance d into the sample is

$$\varepsilon(\rho,z,t)=\left[\frac{dE}{dx}\right]_{\rm eff}\frac{1}{\pi\bar{r}^2}\exp(-\rho^2/\bar{r}^2)\times\frac{1}{2}\left[\operatorname{erf}\left[\frac{d-z}{\bar{r}}\right]+\operatorname{erf}\left[\frac{z}{\bar{r}}\right]\right]\ , \tag{2}$$

where $\bar{r}^2=4\kappa t$, $(dE/dx)_{\rm eff}$ is the energy per path length from the sources, and ρ and z are defined in Fig. 1. The force acting on a part of the solid is given by the gradient of the energy density. For the track normal to the surface of the solid the component of the momentum normal to the surface, p_z, given to a part of the material is obtained by integrating the force over time,[1-3]

$$p_z(\rho,z)=\int_0^\infty \mathbf{F}_z dt=\frac{\beta}{n_M}\int_0^\infty -\nabla\varepsilon(\rho,z,t)\cdot\hat{z}dt=r_cp_c\left[\frac{1}{\sqrt{z^2+\rho^2}}-\frac{1}{\sqrt{(d-z)^2+\rho^2}}\right]\ , \tag{3}$$

where β is a material-dependent constant and n_M is the molecular number density. Here the momentum is written in terms of the parameters r_c and p_c related to the ejection process, where $r_c=\beta(dE/dx)_{\rm eff}/(4\pi\kappa n_M p_c)\propto n_m^{-2/3}U^{-1}(dE/dx)_{\rm eff}$, U is the cohesive energy, and p_c is the critical impulse for ejection. The ejection of a part of the solid is assumed to be determined by $p_z>p_c$. For the case of an infinite line source, it is seen from Eq. (3) that a hemisphere with radius r_c satisfies the ejection criterion $p_z>p_c$ and is therefore ejected. This gives a scaling of the ejection yield as $(dE/dx)^3_{\rm eff}$.[1] This dependence has also been observed in molecular-dynamics calculations.[2,3,5] Also other aspects of the model (e.g., sample thickness dependence, angular and velocity distribution of ejecta, shapes of craters in the solid, etc.) have been compared with molecular-dynamics simulations.[2,3]

If the deposited energy is homogeneously distributed inside a cylinder of radius $\bar{\rho}_0$, the component of the momentum normal to the surface received by a part of the solid is now given by a sum of contributions of "tracks" distributed uniformly over the cylinder. Thereby, using Eq. (3) is is found that

$$p_z(\rho,z)=\frac{p_cr_c}{\pi\bar{\rho}_0^2}\left[\int_0^{\bar{\rho}_0}\int_0^{2\pi}\frac{\rho_0 d\rho_0 d\varphi}{\sqrt{z^2+\rho^2+\rho_0^2-2\rho\rho_0\cos\varphi}}-\int_0^{\bar{\rho}_0}\int_0^{2\pi}\frac{\rho_0 d\rho_0 d\varphi}{\sqrt{(d-z)^2+\rho^2+\rho_0^2-2\rho\rho_0\cos\varphi}}\right]\ , \tag{4}$$

where ρ_0 and φ is the position of a contributing "track" making up the cylinder. In Fig. 1 the part of the solid receiving sufficient momentum for ejection is indicated when calculated from Eq. (4) for infinite sample thickness d using the criterion that $p_z>p_c$. Figure 2 shows the ejection yield, the volume of material receiving sufficient momentum times the molecular number density, as a function of the parameter r_c, which is proportional to

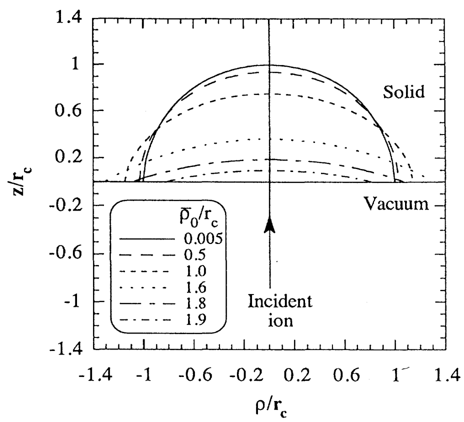

FIG. 1. The ejected part of the solid for different track widths.

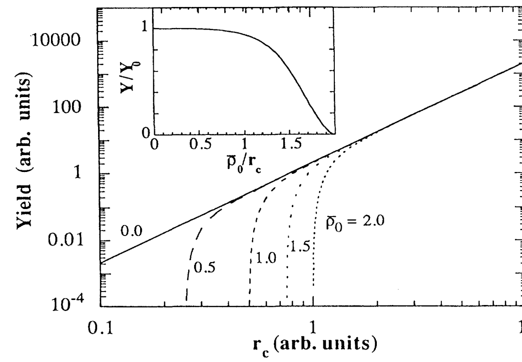

FIG. 2. Ejection yield as a function of the critical radius for ejection $r_c \propto (dE/dx)_{\rm eff}$. The inset shows the ejection yield Y normalized to the ejection yield for $\bar{\rho}_0=0$, $Y_0=2\pi/3r_c^3$, as a function of $\bar{\rho}_0/r_c$.

$(dE/dx)_{\rm eff}$ for infinite sample thickness. From this it is seen that the threshold for the yield occurs at $r_c=\bar{\rho}_0/2$. That is, although the same $(dE/dx)_{\rm eff}$ is deposited it is now too dilute to transfer sufficient momentum for ejection to any part of the solid. It is also seen from these figures that the dependence of the yield on $(dE/dx)_{\rm eff}$ deviates noticeably from the third power *only* for $r_c<0.8\bar{\rho}_0$. Larger $\bar{\rho}_0$ corresponds to ejection only from inside the excited track. This shows that the assumption $r_c \gg \bar{\rho}_0$ made in Ref. 1 for observing the roughly cubic dependence on $(dE/dx)_{\rm eff}$ (i.e., r_c) is unnecessarily strong. In Refs. 2 and 3 the molecular-dynamics simulations were done for $r_c>\bar{\rho}_0$ and $Y\propto(dE/dx)_{\rm eff}^3$ was observed. The simulations by Cui and Johnson[5] were done close to the threshold and the yield varied as the third power of the energy loss only for the highest yields in agreement with Fig. 2. Urbassek, Kafemann, and Johnson[6] observed in their simulations that the yield increased as $(dE/dx)_{\rm eff}$ to a power of 3 to 4 only for low energy loss but approximately linearly with $(dE/dx)_{\rm eff}$ for high energy loss. They also found that mainly the excited part of the solid is ejected even at high energy deposition which results in a much different crater shape from that predicted by our continuum mechanical model. They suggest that the pressure pulse, as defined here, dominates the ejection only for low excitation densities in Ref. 6, and in this region their crater shape is similar to that for $\bar{\rho}_0/r_c \approx 1.6$ in Fig. 1. Whereas the radial pressure ejects the walls, as observed in Refs. 2 and 3, this is not observed in Ref. 6 in which the material properties and the nature of the energy deposition differ.

For a finite sample thickness the yield increases slower than $(dE/dx)_{\rm eff}^3$ for a track with no extension.[3] The dependence of the yield on $(dE/dx)_{\rm eff}$ is not influenced by the width of the track for high energy deposition (i.e., $r_c>\bar{\rho}_0$). A threshold for the yield occurs at $r_c=\bar{\rho}_0/[2(1-\sqrt{d^2/\bar{\rho}_0^2+1}+d/\bar{\rho}_0)]$. This equation can be rewritten to give the threshold thickness d for material ejection at a given energy deposition: $d/r_c=(\bar{\rho}_0/r_c)^2(4-\bar{\rho}_0/r_c)/(8-4\bar{\rho}_0/r_c)$. Close to the threshold when the yield is small the pressure pulse model is not applicable and a statistical model has to be used.[7]

It is concluded that finite track width influences the ejection yield by introducing a threshold for material ejection only when a large part of the ejected material originates from within the track.

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